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A unified approach to preserve structure and thermodynamics in a coarse-grained model of aqueous mixtures PRITAM GANGULY, Center of Smart Interfaces, TU Darmstadt, Germany, DEBASHISH MUKHERJI, CHRISTOPH JUNGHANS, Max Planck Institute for Polymer Research, Mainz, Germany, NICO VAN DER VEGT, Center of Smart Interfaces, TU Darmstadt, Germany — Biological organizations depend on a sensitive balance of noncovalent interactions, in particular also those involving interactions of small molecules, including inorganic salts and urea, with biomolecules in aqueous solution. Computer simulations of these types of systems require simple-yet-specific models in order to cover all relevant time and length scales. We present a method to systematically coarse-grain liquid mixtures using Kirkwood-Buff theory of solution combined with an iterative Boltzmann inversion technique that infers single-site interaction potentials for the solution components from the pair correlation functions. Our method preserves both the solution structure at pair level and variations of solution components' chemical potentials with compositions within a unified coarse-graining framework. To test the robustness of our approach, we simulated urea-water and benzene-water systems over a wide-range of concentrations. We also observe the coarse-grained potentials to be reasonably transferable with varying concentrations.

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